

Biphenyl
92-52-4 | DTXSID4020161

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.70

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 8.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Azulene</div> <div>Measured: 3.20</div> <div>Predicted: 2.94</div>	<div>Image not found</div> <div>Naphthalene</div> <div>Measured: 3.30</div> <div>Predicted: 3.00</div>	<div>Image not found</div> <div>Biphenyl</div> <div>Measured: 4.01</div> <div>Predicted: 3.70</div>
<div>Image not found</div> <div>Acenaphthene</div> <div>Measured: 3.92</div> <div>Predicted: 2.47</div>	<div>Image not found</div> <div>9H-Xanthene</div> <div>Measured: 4.23</div> <div>Predicted: 3.06</div>	